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Hybrid simulation of neutral gas interacting with a plasma *

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Plasma in contact with a material surface is neutralized and recycled as a gas that in turn interacts with the plasma. The neutral gas may be in a kinetic regime (long mean free path) in some regions and in a fluid regime (short mean free path) elsewhere. In order to model this situation, we imagine the neutral gas as the superposition of two populations, one fluid and one kinetic, with transfer terms coupling the two populations. We model these populations by coupling together a plasma fluid code, B2.5,[1] and a neutral Monte Carlo code, Degas 2.[2] The coupling terms conserve mass, momentum, and energy, and are chosen so that fluid neutrals are converted to kinetic neutrals where their mean free path is long and vice versa. In this scheme, self collisions are never a dominant term in the Monte Carlo code may be treated by a simplified BGK model.

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[1]B. J. Braams, Radiative Divertor Modelling for ITER and TPX, Contrib. Plasma Phys. **36**, 276–281 (1996)

[2]D. P. Stotler and C. F. F. Karney, Neutral Gas Transport Modeling with Degas 2, Contrib. Plasma Phys. **34**, 392–397 (1994).

Introduction

A power producing fusion reactor requires that the power and ash be continually removed from the device. This requires a design where hot plasma recombines either on a material surface or in a gas blanket usually in a region of the device call a "divertor" which is magnetically separated from the hot fusing plasma.

In the divertor, the plasma is strongly coupled to a population of neutral atoms and molecules through a variety of reactions: ionization, recombination, charge exchange, etc.

In this paper, we describe:

- Degas 2, a Monte Carlo code which models the transport of neutrals in the kinetic regime;
- A proposed coupling of Degas 2 to a plasma fluid code, B2, in order to describe the transport of models in the fluid-kinetic transition.

Degas 2

Degas 2 is a comprehensive Monte Carlo modeling code tailored to the needs of neutral transport in plasma devices. Key features are:

- Flexible three-dimensional geometry. The problem domain is broken down into cells which are bounded by quadratic surfaces. There is a "pseudo-convexity" requirement on these cells which makes particle tracking faster. However, the cells can be combined together to describe arbitrary shapes accurately.

- Fast tracking algorithms. The intersection of a track with a cell face to be computed in time $O(N)$ where N is the number of faces in a cell

- Flexible handling of particles, reactions, material surfaces, and scoring. These are all specified at runtime by means of tables.

- Operation on parallel machines via PVM (and MPI soon).

- Written in FWEB (`http://w3.pppl.gov/~krommes/fweb_toc.html`) which simplifies coding and documenation. This produces either formatted documentation or code (either standard Fortran 90 or Fortran 77 with pointer extensions, for dynamic memory allocation). FWEB source code is 40k lines. Fortran 90 code is 70k lines.

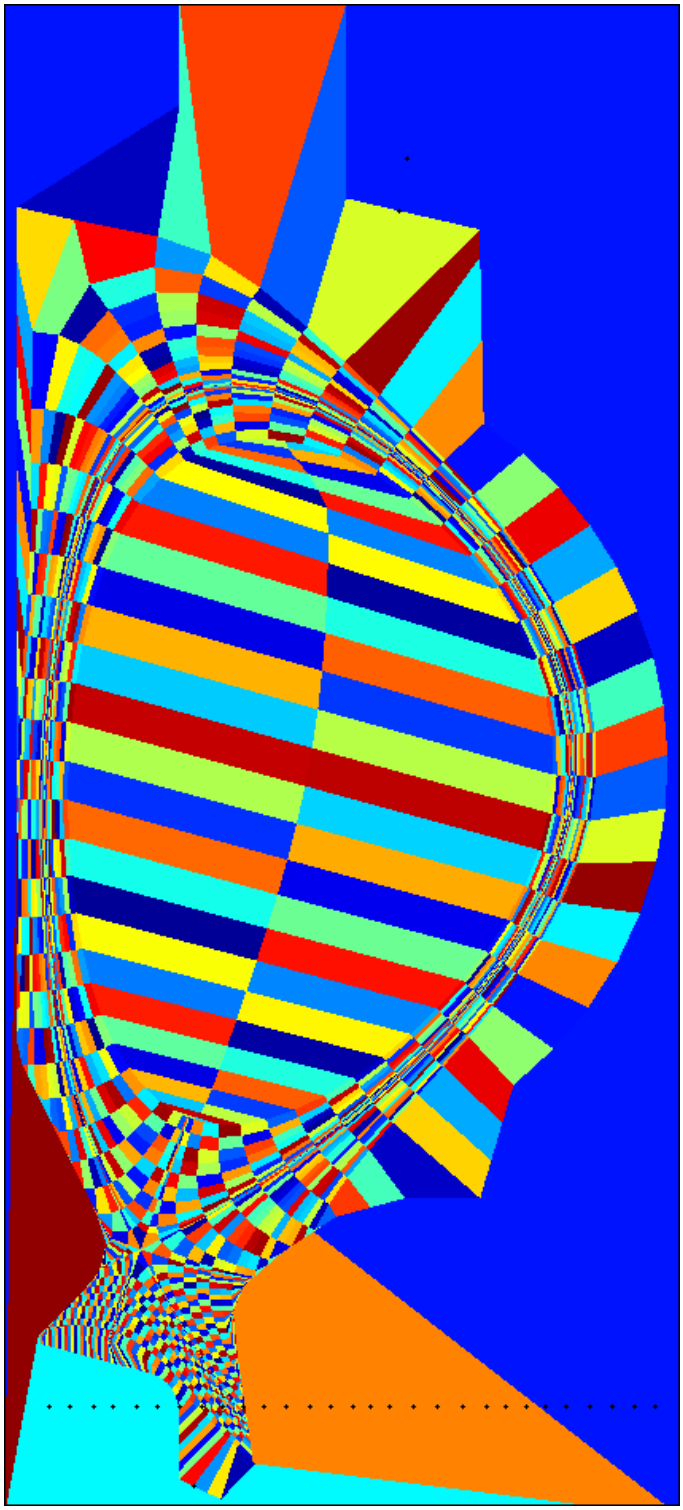
- NETCDF is used for most file I/O.

- Standard tools (make, CVS) are used to maintain the code.

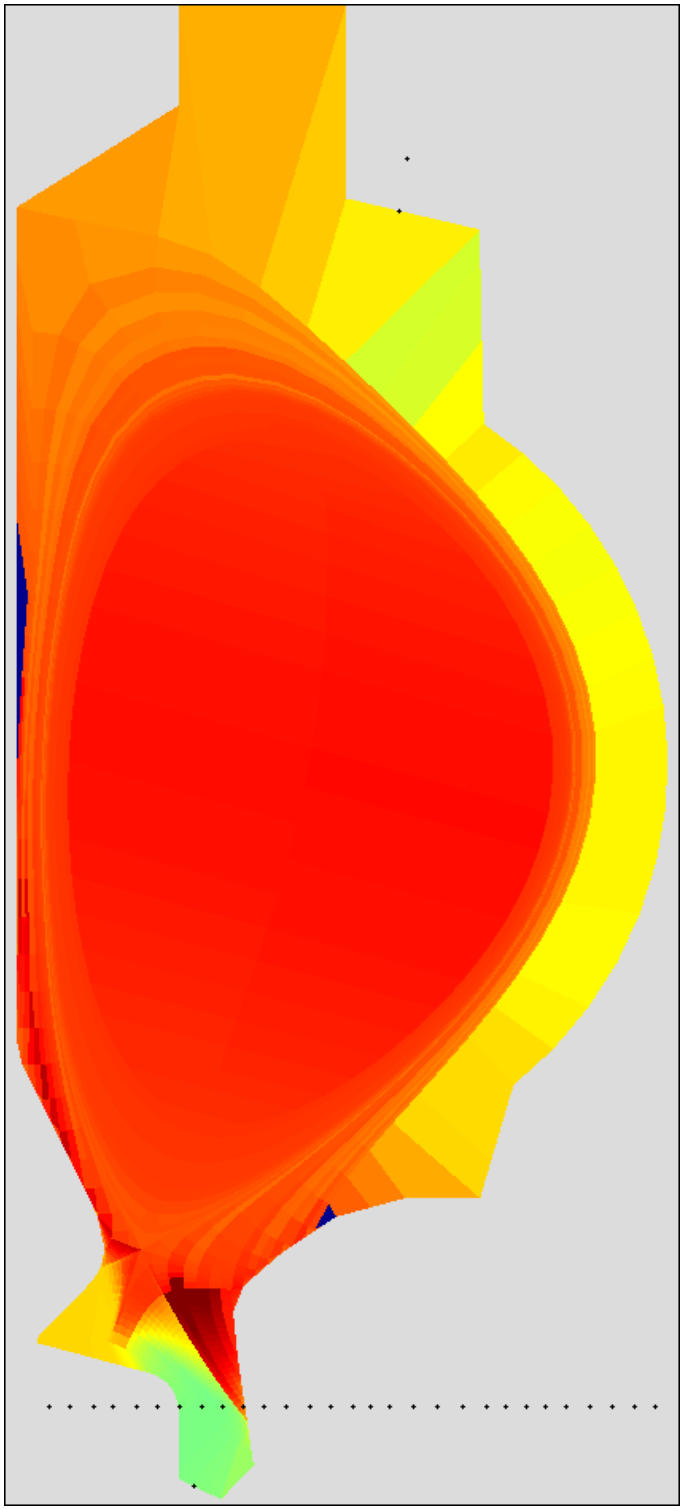
- Uses a portable random number generator which produces the same random sequences on different architectures. In addition, repeatable independent threads of random numbers can be produced in multiprocessor applications.

Following figures show sample results for a simulation of D and D_2 transport in the CMOD fusion device at MIT.

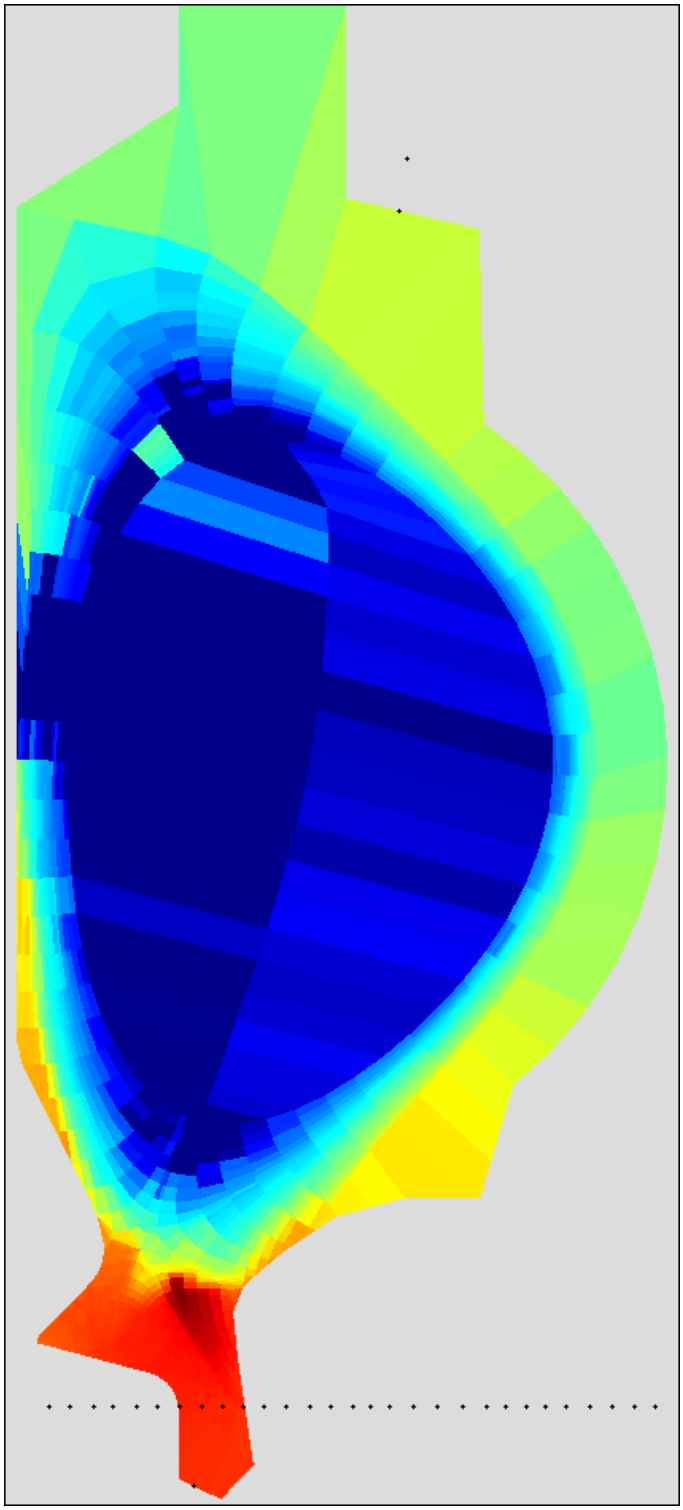
Geometry



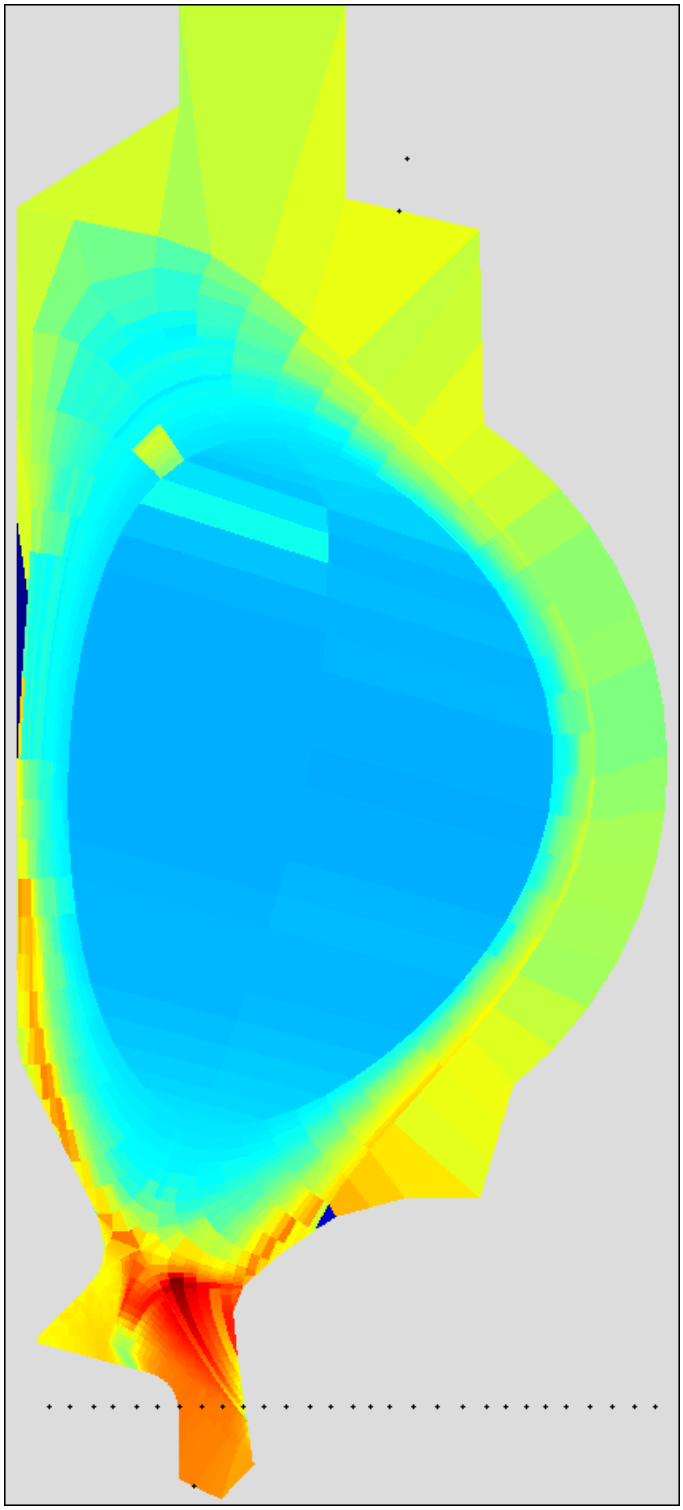
electron density (input)



deuterium atom density



D_α line emission



Hybrid modeling of neutrals

In many cases of interest in the divertors of fusion devices, the neutral density may become high enough that the fluid approximation is valid ($\lambda \gg L$) and the transport can be accurately computed from suitable fluid equations, e.g., the Navier-Stokes equations. The Monte Carlo method, on the other hand, is becomes a very inefficient in this regime.

Unfortunately, a kinetic treatment is still required in some regimes ($\lambda \ll L$) either because the neutral density is low, e.g., in the hot plasma, or because the scale length is short, e.g., in the ionization front or close to a material surface. In this region the full Boltzmann equations need to be solved, e.g., by the Monte Carlo method.

One possible way of treating this situation is to divide the domain up into fluid and kinetic subdomains and solve the appropriate equations in each subdomain with suitable boundary terms. We reject this because of the complexity of setting up the domains and because of the domain boundaries will need to be adjusted during the course of the computation.

Instead we choose to distinguish two classes of neutrals: "kinetic" (to be computed via a Monte Carlo method) and "fluid" (to be computed via fluid equation). Both classes coexist throughout the problem domain. Let us denote the two classes by $\mathrm{H}_{\mathrm{kin}}$ and H_{fl}.
The two classes of neutral are coupled by:

- Collisions. For example, neutral-neutral collosions appear in the Boltzmann equation as

  $$C(\mathrm{H}_{\mathrm{kin}}, \mathrm{H}_{\mathrm{kin}}) + C(\mathrm{H}_{\mathrm{kin}}, \mathrm{H}_{\mathrm{fl}})$$

  (also kinetic neutrals interact with the plasma, a multi-species fluid, via charge exchange, ionization, recombination, ...).

- Transfers. For example, where $\lambda \gg L$ we have the "condensation" reaction

  $$\mathrm{H}_{\mathrm{fl}} \to \mathrm{H}_{\mathrm{kin}}$$

  which proceeds with a rate ν_c and where $\lambda \ll L$ we have the "evaporation" reaction

  $$\mathrm{H}_{\mathrm{kin}} \to \mathrm{H}_{\mathrm{fl}}$$

  which proceeds with a rate ν_e. Here ν_c (resp. ν_e) is a increasing (resp. decreasing) function of λ/L. These processes appear as sources and sinks in the fluid and Boltzmann equations and are analogous to processes of recombination and ionization already treated in the coupled fluid plasma-Monte Carlo neutral codes

Key Features

- A natural extension of existing modeling efforts via fluid-Monte Carlo codes.
- Adaptive — the ratio $n_{\mathrm{H_{fl}}}/n_{\mathrm{H_{kin}}}$ adjusts to local conditions.
- Nearly optimal — Monte Carlo particles are concentrated in the kinetic regions where they are needed; there is not much penalty in solving the fluid equations everywhere.
- The collision term $C(\mathrm{H_{kin}}, \mathrm{H_{kin}})$ is never dominant and may be treated is an approximate manner (via a BGK collision operator). This preserves the linearity of the Monte Carlo equations.

An example

Consider fast ions diffusion in one dimension in a fixed electron background. This is "exactly" descibed by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \nu\frac{\partial}{\partial v}\left(v_t^2\frac{\partial f}{\partial v} + vf\right) + S_{\text{kin}},$$

where $v_t^2 = T_e/m_i$.
We may derive fluid equations using Chapman Engskog procedure for $\lambda = v_t/\nu \ll L$

$$f_0 = n(x,t)\frac{\exp(-v^2/(2v_t^2))}{\sqrt{2\pi}v_t},$$

$$f_1 = -f_0\frac{v}{\nu}\frac{1}{n}\frac{\partial n}{\partial x}.$$

The resulting fluid equation is a simple diffusion equation

$$\frac{\partial n}{\partial t} = \frac{v_t^2}{\nu}\frac{\partial^2 n}{\partial x^2} + S_{\text{fl}}.$$

(There is only one fluid equation since the collision operator only conserves density.)

- Proposed scheme involves solving both the Boltzmann and fluid equations.
- Number conservation for the combined system give

$$S_{\mathrm{fl}} + \int S_{\mathrm{kin}}\, dv = 0.$$

- We might choose

$$S_{\mathrm{kin}} = -\nu_e f + \nu_c f_0.$$

- Coupling can be conveniently investigated in this example, since both equations have analytic solutions (via Green's functions).

A copy of this poster will appear shortly at `http://w3.pppl.gov/degas2`.